Microcrystallography and Mapping Radiation Damage with a 1-micron Beam at GM/CA-CAT

Robert F. Fischetti GM/CA-CAT, Biosciences Division, Argonne National Laboratory, Argonne, 60439

Microcrystallography enables structure determination from crystals with micron-dimensions by reducing the size of the beam to that of the crystal, thereby reducing the background and improving the signal-to-noise of the data. Micro-beams are now used as a probe to create diffraction quality maps of larger crystals allowing selection of the best parts of the crystal for data collection. The effects of radiation damage can be minimized by walking a micro-beam along rod shaped crystals of small cross section and collecting partial data sets that can easily be merged into a full data set. To meet the growing demand we continue to develope hardware and software for micro-crystallography. Our "mini-beam" collimators have been redesigned to improve reliability and robustness. New quad-collimators provide 5, 10 and 20 microns beams as well as the full focused beam on demand. An active beamstop based on the photoelectric effect has been developed providing real-time measurements of the intensity transmitted through the sample. A goniometer with a 1-micron peak-to-peak sphere of confusion that can carry sample position stages with nanometer resolution and repeatability has been designed and implemented.

For the atoms biologically relevant to MX, the X-ray cross section tends to be dominated by the photoelectric effect. Most of the X-rays energy is converted into kinetic energy of the photoelectron. As the photoelectron traverses the crystal it gradually loses more and more energy until it is recaptured. This re-deposition of energy is thought to be one of the major sources of radiation damage to the crystal. Several papers in the past few years have carried out both calculations and Monte Carlo simulations of photoelectron trajectory and energy loss (1,2,3). These papers outline schemes for reducing radiation damage by using very small X-ray beams.

In this talk I will present the current status of microcrystallography at GM/CA-CAT and our future plans. Data will also be presented addressing the distribution of radiation induced damage about a 1-micron beam and how it compares to the theoretical calculations.

- 1) Nave, C. and Hill, M. A. (2005). J Sync. Rad. 12, 299-303.
- 2) Cowan, J. and Nave, C. (2008) J Sync. Rad. 15, 458-462
- 3) Stern, E., Yacoby, Y., Seidler, G., Nagle, K., Prange, M., Sorini, A. Rehr, J. and Joachimiak, A. (2009) *Acta Cryst.* D65, 366-374